Appendix A
Computation of Principal Components

This Appendix is the only part of the book that has shrunk compared to the first edition, where it consisted of two sections. The first described efficient methods for deriving PCs, that is efficient techniques from numerical analysis for calculating eigenvectors and eigenvalues of positive semi-definite matrices; the second section discussed the facilities for computing PCs, and performing related analyses, which were then available in five of the best known statistical computer packages.

The first topic has been updated in this edition and some general comments on the second topic are included. However much of the detail on the latter topic has been removed from this edition, mainly because such material rapidly becomes out of date. This is readily illustrated by two quotations from the first edition.

> Despite the likelihood that personal computers will become the main tool for ... users of PCA ... [it] is still usually carried out on mainframe computers ... [T]he author has no experience yet of PCA on personal computers.

> MINITAB does not have any direct instructions for finding PCs.

Five packages were described in the first edition—BMDP, GENSTAT, MINITAB, SAS and SPSS^X. Since then a number a new packages or languages have appeared. Perhaps the biggest change is the greatly expanded use by statisticians of S-PLUS and its 'open source' relative R. The MATLAB software should also be mentioned. Although it is not primarily a statistical package, it has found increasing favour among statisticians as a

programming environment within which new statistical techniques can be implemented. PCA is also included in some neural network software.

All the main statistical software packages incorporate procedures for finding the basic results of a PCA. There are some variations in output, such as the choice of normalization constraints used for the vectors of loadings or coefficients. This can cause confusion for the unwary user (see Section 11.1), who may also be confused by the way in which some software erroneously treats PCA as a special case of factor analysis (see Chapter 7). However, even with this misleading approach, numerically correct answers are produced by all the major statistical software packages, and provided that the user is careful to ensure that he or she understands the details of how the output is presented, it is usually adequate to use whichever software is most readily available.

Most statistical packages produce the basic results of a PCA satisfactorily, but few provide much in the way of extensions or add-ons as standard features. Some allow (or even encourage) rotation, though not necessarily in a sufficiently flexible manner to be useful, and some will display biplots. With most it is fairly straightforward to use the output from PCA in another part of the package so that PC regression, or discriminant or cluster analysis using PCs instead of the measured variables (see Chapters 8 and 9) are easily done. Beyond that, there are two possibilities for many of the extensions to PCA. Either software is available from the originator of the technique, or extra functions or code can be added to the more flexible software, such as S-PLUS or R.

A.1 Numerical Calculation of Principal Components

Most users of PCA, whether statisticians or non-statisticians, have little desire to know about efficient algorithms for computing PCs. Typically, a statistical program or package can be accessed that performs the analysis automatically. Thus, the user does not need to write his or her own programs; often the user has little or no interest in whether or not the software available performs its analyses efficiently. As long as the results emerge, the user is satisfied.

However, the type of algorithm used can be important, in particular if some of the last few PCs are of interest or if the data set is very large. Many programs for PCA are geared to looking mainly at the first few PCs, especially if PCA is included only as part of a factor analysis routine. In this case, several algorithms can be used successfully, although some will encounter problems if any pairs of the eigenvalues are very close together. When the last few or all of the PCs are to be calculated, difficulties are more likely to arise for some algorithms, particularly if some of the eigenvalues are very small.

Finding PCs reduces to finding the eigenvalues and eigenvectors of a positive-semidefinite matrix. We now look briefly at some of the possible algorithms that can be used to solve such an eigenproblem.

The Power Method

A form of the power method was described by Hotelling (1933) in his original paper on PCA, and an accelerated version of the technique was presented in Hotelling (1936). In its simplest form, the power method is a technique for finding the largest eigenvalue and the corresponding eigenvector of a $(p \times p)$ matrix $\mathbf{T}$. The idea is to choose an initial p-element vector $\mathbf{u}_0$, and then form the sequence

$$\begin{aligned}
\mathbf{u}_1 &= \mathbf{T}\mathbf{u}_0 & \\
\mathbf{u}_2 &= \mathbf{T}\mathbf{u}_1 &= \mathbf{T}^2\mathbf{u}_0 \\
&\ \ \vdots & \vdots \\
\mathbf{u}_r &= \mathbf{T}\mathbf{u}_{r-1} &= \mathbf{T}^r\mathbf{u}_0 \\
&\ \ \vdots & \vdots
\end{aligned}$$

If $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_p$ are the eigenvectors of $\mathbf{T}$, then they form a basis for p-dimensional space, and we can write, for arbitrary $\mathbf{u}_0$,

$$\mathbf{u}_0 = \sum_{k=1}^{p} \kappa_k \boldsymbol{\alpha}_k$$

for some set of constants $\kappa_1, \kappa_2, \ldots, \kappa_p$. Then

$$\mathbf{u}_1 = \mathbf{T}\mathbf{u}_0 = \sum_{k=1}^{p} \kappa_k \mathbf{T}\boldsymbol{\alpha}_k = \sum_{k=1}^{p} \kappa_k \lambda_k \boldsymbol{\alpha}_k,$$

where $\lambda_1, \lambda_2, \ldots, \lambda_p$ are the eigenvalues of $\mathbf{T}$. Continuing, we get for $r = 2, 3, \ldots$

$$\mathbf{u}_r = \sum_{k=1}^{p} \kappa_k \lambda_k^r \boldsymbol{\alpha}_k$$

and

$$\frac{\mathbf{u}_r}{(\kappa_1 \lambda_1^r)} = \left(\boldsymbol{\alpha}_1 + \frac{\kappa_2}{\kappa_1}\left(\frac{\lambda_2}{\lambda_1}\right)^r \boldsymbol{\alpha}_2 + \cdots + \frac{\kappa_p}{\kappa_1}\left(\frac{\lambda_p}{\lambda_1}\right)^r \boldsymbol{\alpha}_p \right).$$

Assuming that the first eigenvalue of $\mathbf{T}$ is distinct from the remaining eigenvalues, so that $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_p$, it follows that a suitably normalized version of $\mathbf{u}_r \to \boldsymbol{\alpha}_1$ as $r \to \infty$. It also follows that the ratios of corresponding elements of $\mathbf{u}_r$ and $\mathbf{u}_{r-1} \to \lambda_1$ as $r \to \infty$.

The power method thus gives a simple algorithm for finding the first (largest) eigenvalue of a covariance or correlation matrix and its corresponding eigenvector, from which the first PC and its variance can be

derived. It works well if $\lambda_1 \gg \lambda_2$, but converges only slowly if λ_1 is not well separated from λ_2. Speed of convergence also depends on the choice of the initial vector $\mathbf{u}_0$; convergence is most rapid if $\mathbf{u}_0$ is close to $\boldsymbol{\alpha}_1$,

If $\lambda_1 = \lambda_2 > \lambda_3$, a similar argument to that given above shows that a suitably normalized version of $\mathbf{u}_r \to \boldsymbol{\alpha}_1 + (\kappa_2/\kappa_1)\boldsymbol{\alpha}_2$ as $r \to \infty$. Thus, the method does not lead to $\boldsymbol{\alpha}_1$, but it still provides information about the space spanned by $\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$. Exact equality of eigenvalues is extremely unlikely for *sample* covariance or correlation matrices, so we need not worry too much about this case.

Rather than looking at all $\mathbf{u}_r$, $r = 1, 2, 3, \ldots$, attention can be restricted to $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_4, \mathbf{u}_8, \ldots$ (that is $\mathbf{T}\mathbf{u}_0, \mathbf{T}^2\mathbf{u}_0, \mathbf{T}^4\mathbf{u}_0, \mathbf{T}^8\mathbf{u}_0, \ldots$) by simply squaring each successive power of $\mathbf{T}$. This accelerated version of the power method was suggested by Hotelling (1936). The power method can be adapted to find the second, third, ...PCs, or the last few PCs (see Morrison, 1976, p. 281), but it is likely to encounter convergence problems if eigenvalues are close together, and accuracy diminishes if several PCs are found by the method. Simple worked examples for the first and later components can be found in Hotelling (1936) and Morrison (1976, Section 8.4) .

There are various adaptations to the power method that partially overcome some of the problems just mentioned. A large number of such adaptations are discussed by Wilkinson (1965, Chapter 9), although some are not directly relevant to positive-semidefinite matrices such as covariance or correlation matrices. Two ideas that *are* of use for such matrices will be mentioned here. First, the origin can be shifted, that is the matrix $\mathbf{T}$ is replaced by $\mathbf{T} - \rho\mathbf{I}_p$, where $\mathbf{I}_p$ is the identity matrix, and ρ is chosen to make the ratio of the first two eigenvalues of $\mathbf{T} - \rho\mathbf{I}_p$ much larger than the corresponding ratio for $\mathbf{T}$, hence speeding up convergence.

A second modification is to use inverse iteration (with shifts), in which case the iterations of the power method are used but with $(\mathbf{T} - \rho\mathbf{I}_p)^{-1}$ replacing $\mathbf{T}$. This modification has the advantage over the basic power method with shifts that, by using appropriate choices of ρ (different for different eigenvectors), convergence to *any* of the eigenvectors of $\mathbf{T}$ can be achieved. (For the basic method it is only possible to converge in the first instance to $\boldsymbol{\alpha}_1$ or to $\boldsymbol{\alpha}_p$.) Furthermore, it is not necessary to explicitly calculate the inverse of $\mathbf{T}-\rho\mathbf{I}_p$, because the equation $\mathbf{u}_r = (\mathbf{T}-\rho\mathbf{I}_p)^{-1}\mathbf{u}_{r-1}$ can be replaced by $(\mathbf{T} - \rho\mathbf{I}_p)\mathbf{u}_r = \mathbf{u}_{r-1}$. The latter equation can then be solved using an efficient method for the solution of systems of linear equations (see Wilkinson, 1965, Chapter 4). Overall, computational savings with inverse iteration can be large compared to the basic power method (with or without shifts), especially for matrices with special structure, such as tridiagonal matrices. It turns out that an efficient way of computing PCs is to first transform the covariance or correlation matrix to tridiagonal form using, for example, either the Givens or Householder transformations (Wilkinson, 1965, pp. 282, 290), and then to implement inverse iteration with shifts on this tridiagonal form.

There is one problem with shifting the origin that has not yet been mentioned. This is the fact that to choose efficiently the values of ρ that determine the shifts, we need some preliminary idea of the eigenvalues of $\mathbf{T}$. This preliminary estimation can be achieved by using the method of bisection, which in turn is based on the Sturm sequence property of tridiagonal matrices. Details will not be given here (see Wilkinson, 1965, pp. 300–302), but the method provides a quick way of finding approximate values of the eigenvalues of a tridiagonal matrix. In fact, bisection could be used to find the eigenvalues to any required degree of accuracy, and inverse iteration implemented solely to find the eigenvectors.

Two major collections of subroutines for finding eigenvalues and eigenvectors for a wide variety of classes of matrix are the EISPACK package (Smith et al., 1976), which is distributed by IMSL, and parts of the NAG library of subroutines. In both of these collections, there are recommendations as to which subroutines are most appropriate for various types of eigenproblem. In the case where only a few of the eigenvalues and eigenvectors of a real symmetric matrix are required (corresponding to finding just a few of the PCs for a covariance or correlation matrix) both EISPACK and NAG recommend transforming to tridiagonal form using Householder transformations, and then finding eigenvalues and eigenvectors using bisection and inverse iteration respectively. NAG and EISPACK both base their subroutines on algorithms published in Wilkinson and Reinsch (1971), as do the 'Numerical Recipes' for eigensystems given by Press et al. (1992, Chapter 11).

The QL Algorithm

If all of the PCs are required, then methods other than those just described may be more efficient. For example, both EISPACK and NAG recommend that we should still transform the covariance or correlation matrix to tridiagonal form, but at the second stage the so-called QL algorithm should now be used, instead of bisection and inverse iteration. Chapter 8 of Wilkinson (1965) spends over 80 pages describing the QR and LR algorithms (which are closely related to the QL algorithm), but only a very brief outline will be given here.

The basic idea behind the QL algorithm is that any non-singular matrix $\mathbf{T}$ can be written as $\mathbf{T} = \mathbf{QL}$, where $\mathbf{Q}$ is orthogonal and $\mathbf{L}$ is lower triangular. (The $\mathbf{QR}$ algorithm is similar, except that $\mathbf{T}$ is written instead as $\mathbf{T} = \mathbf{QR}$, where $\mathbf{R}$ is upper triangular, rather than lower triangular.) If $\mathbf{T}_1 = \mathbf{T}$ and we write $\mathbf{T}_1 = \mathbf{Q}_1\mathbf{L}_1$, then $\mathbf{T}_2$ is defined as $\mathbf{T}_2 = \mathbf{L}_1\mathbf{Q}_1$. This is the first step in an iterative procedure. At the next step, $\mathbf{T}_2$ is written as $\mathbf{T}_2 = \mathbf{Q}_2\mathbf{L}_2$ and $\mathbf{T}_3$ is defined as $\mathbf{T}_3 = \mathbf{L}_2\mathbf{Q}_2$. In general, $\mathbf{T}_r$ is written as $\mathbf{Q}_r\mathbf{L}_r$ and $\mathbf{T}_{r+1}$ is then defined as $\mathbf{L}_r\mathbf{Q}_r$, $r = 1, 2, 3, \ldots$, where $\mathbf{Q}_1$, $\mathbf{Q}_2$, $\mathbf{Q}_3, \ldots$ are orthogonal matrices, and $\mathbf{L}_1$, $\mathbf{L}_2$, $\mathbf{L}_3, \ldots$ are lower triangular. It can be shown that $\mathbf{T}_r$ converges to a diagonal matrix, with the eigenvalues

of **T** in decreasing absolute size down the diagonal. Eigenvectors can be found by accumulating the transformations in the QL algorithm (Smith et al., 1976, p. 468).

As with the power method, the speed of convergence of the QL algorithm depends on the ratios of consecutive eigenvalues. The idea of incorporating shifts can again be implemented to improve the algorithm and, unlike the power method, efficient strategies exist for finding appropriate shifts that do not rely on prior information about the eigenvalues (see, for example, Lawson and Hanson (1974, p. 109)). The QL algorithm can also cope with equality between eigenvalues.

It is probably fair to say that the algorithms described in detail by Wilkinson (1965) and Wilkinson and Reinsch (1971), and implemented in various IMSL and NAG routines, have stood the test of time. They still provide efficient ways of computing PCs in many circumstances. However, we conclude the Appendix by discussing two alternatives. The first is implementation *via* the singular value decomposition (SVD) of the data matrix, and the second consists of the various algorithms for PCA that have been suggested in the neural networks literature. The latter is a large topic and will be summarized only briefly.

One other type of algorithm that has been used recently to find PCs is the EM algorithm (Dempster et al., 1977). This is advocated by Tipping and Bishop (1999a,b) and Roweis (1997), and has its greatest value in cases where some of the data are missing (see Section 13.6).

Singular Value Decomposition

The suggestion that PCs may best be computed using the SVD of the data matrix (see Section 3.5) is not new. For example, Chambers (1977, p. 111) talks about the SVD providing the best approach to computation of principal components and Gnanadesikan (1977, p. 10) states that '...the recommended algorithm for ... obtaining the principal components is either the ... QR method ... or the singular value decomposition.' In constructing the SVD, it turns out that similar algorithms to those given above can be used. Lawson and Hanson (1974, p. 110) describe an algorithm (see also Wilkinson and Reinsch (1971)) for finding the SVD, which has two stages; the first uses Householder transformations to transform to an upper bidiagonal matrix, and the second applies an adapted QR algorithm. The method is therefore not radically different from that described earlier.

As noted at the end of Section 8.1, the SVD can also be useful in computations for regression (Mandel, 1982; Nelder, 1985), so the SVD has further advantages if PCA is used in conjunction with regression. Nash and Lefkovitch (1976) describe an algorithm that uses the SVD to provide a variety of results for regression, as well as PCs.

Another point concerning the SVD is that it provides simultaneously not only the coefficients and variances for the PCs, but also the scores of each

observation on each PC, and hence all the information that is required to construct a biplot (see Section 5.3). The PC scores would otherwise need to be derived as an extra step after calculating the eigenvalues and eigenvectors of the covariance or correlation matrix $\mathbf{S} = \frac{1}{n-1}\mathbf{X}'\mathbf{X}$.

The values of the PC scores are related to the eigenvectors of $\mathbf{X}\mathbf{X}'$, which can be derived from the eigenvectors of $\mathbf{X}'\mathbf{X}$ (see the proof of Property G4 in Section 3.2); conversely, the eigenvectors of $\mathbf{X}'\mathbf{X}$ can be found from those of $\mathbf{X}\mathbf{X}'$. In circumstances where the sample size n is smaller than the number of variables p, $\mathbf{X}\mathbf{X}'$ has smaller dimensions than $\mathbf{X}'\mathbf{X}$, so that it can be advantageous to use the algorithms described above, based on the power method or QL method, on a multiple of $\mathbf{X}\mathbf{X}'$ rather than $\mathbf{X}'\mathbf{X}$ in such cases. Large computational savings are possible when $n \ll p$, as in chemical spectroscopy or in the genetic example of Hastie et al. (2000), which is described in Section 9.2 and which has $n = 48$, $p = 4673$. Algorithms also exist for updating the SVD if data arrive sequentially (see for example Berry et al. (1995)).

Neural Network Algorithms

Neural networks provide ways of extending PCA, including some non-linear generalizations (see Sections 14.1.3, 14.6.1). They also give alternative algorithms for estimating 'ordinary' PCs. The main difference between these algorithms and the techniques described earlier in the Appendix is that most are 'adaptive' rather than 'batch' methods. If the whole of a data set is collected before PCA is done and parallel processing is not possible, then batch methods such as the QR algorithm are hard to beat (see Diamantaras and Kung, 1996 (hereafter DK96), Sections 3.5.3, 4.4.1). On the other hand, if data arrive sequentially and PCs are re-estimated when new data become available, then adaptive neural network algorithms come into their own. DK96, Section 4.2.7 note that 'there is a plethora of alternative [neural network] techniques that perform PCA.' They describe a selection of single-layer techniques in their Section 4.2, with an overview of these in their Table 4.1. Different algorithms arise depending on

- whether the first or last few PCs are of interest;
- whether one or more than one PC is required;
- whether individual PCs are wanted or whether subspaces spanned by several PCs will suffice;
- whether the network is required to be biologically plausible.

DK96, Section 4.2.7 treat finding the last few PCs as a different technique, calling it *minor component analysis*.

In their Section 4.4, DK96 compare the properties, including speed, of seven algorithms using simulated data. In Section 4.5 they discuss multi-layer networks.

Neural network algorithms are feasible for larger data sets than batch methods because they are better able to take advantage of developments in computer architecture. DK96, Chapter 8, discuss the potential for exploiting parallel VSLI (very large scale integration) systems, where the most appropriate algorithms may be different from those for non-parallel systems (DK96, Section 3.5.5). They discuss both digital and analogue implementations and their pros and cons (DK96, Section 8.3). Classical eigenvector-based algorithms are not easily parallelizable, whereas neural network algorithms are (DK96 pp. 205–207).

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